CONTENTS

Special Issue: The Electronic Structure and Properties of Molecules, Clusters and Crystals

Preface ..... *ix*
Rudjer Bošković: anticipation of modern science
I. Supek (Zagreb, Yugoslavia) 1
Ab initio calculation of molecular properties
W. Kutzelnigg (Bochum, F.R.G.) 11
Treatment of electron correlations by local operators: a status report
P. Fulde (Stuttgart, F.R.G.) 63
Appraisal of Hermite–Gaussian expansion of hydrogen orbitals by calculation of some one-electron properties
M. Primorac, K. Kovačević and Z.B. Maksić (Zagreb, Yugoslavia) 75
Electron density for atoms from Fues potential within *H–K–S* theory
K. Tkacz and W.S. Ptak (Cracow, Poland) 91
The localized electronegativity group orbital (LEGO): group hardnesses for acids and bases theory
J. Todd and M.A. Whitehead (Montreal, PQ, Canada) 99
Comparison of X-ray and ab initio deformation densities in dimethyl-γ-pyrone and triazine trichloride
Z. Darakjian, W.H. Fink and H. Hope (Davis, CA, U.S.A.) 111
On the effect of conjugation and charge transfer on the polarisability, first and second hyperpolarisabilities of some polyenes and nitropolyenes
M.G. Papadopoulos and J. Waite (Athens, Greece) 121
Electronic structure and properties of molecules in excited states
M. Klessinger (Münster, F.R.G.) 129
MRD-CI quartet potential surfaces for the collinear reactions $N(^4S_u)+N_2(X^1\Sigma_g^+, A^3\Sigma_u^+$, and $B^3\pi_g)$
C. Petrongolo (Sassari, Italy) 135
Conformational analysis and structural determinations from ab initio calculations for chloroacetaldehyde
J.R. Durig, H.V. Phan, T.S. Little (Columbia, SC, U.S.A.) and B.J. van der Veken (Antwerp, Belgium) 143
Conformational analysis and structural determinations from ab initio calculations for vinyl silyl chloride
J.F. Sullivan, M.A. Qtaitat and J.R. Durig (Columbia, SC, U.S.A.) 159
Quantum-chemically supported vibrational analysis of giant molecules: the C_{60} and C_{70} clusters
Z. Slanina (Kobylisy, Czechoslovakia), J.M. Rudziński, M. Togasi and E. Ōsawa (Sapporo, Japan) 169
Ab initio studies of the structure, energetics and vibrational spectra of hydrogen bonded systems
S. Scheiner (Carbondale, IL, U.S.A.) 177
The frequency–bond length correlation in local-mode overtone spectra
B.R. Henry (Guelph, Ont., Canada) and D.J. Swanton (Canberra, Australia) 193
Theoretical *K*-shell photoelectron spectra of H_2CO and C_2H_2
G. Angonoa and J. Schirmer (Heidelberg, F.R.G.) 203
Inner valence photoelectron spectra – from qualitative to quantitative results
W. von Niessen and P. Tomasello (Braunschweig, F.R.G.) 213
Photoelectron spectroscopy study of substituent effect of halogens on the thiophene ring
T. Veszpremi, L. Nyulaszi, G. Zsombok, J. Reffy (Budapest, Hungary), Cvitaš, B. Kovač and L. Klasinc (Zagreb, Yugoslavia) 227

A new method to calculate lifetimes of atomic and molecular autoionizing states
A. Macias, F. Martin, O. Mo, A. Riera and M. Yañez (Madrid, Spain) 235
Excited-state structures of molecules with nearby electronic states
A.K. Chandra (Bangalore, India) 249
Distributed atomic multipole moments and intermolecular potentials: test calculations of the second virial coefficient of the SO_2 molecule
M. Pavlović, F. Sokolić and Z.B. Maksić (Zagreb, Yugoslavia) 265
Growth of small silicon and aluminum clusters
K. Jug (Hannover, F.R.G.) 277
Chemically bound excited clusters
C.A. Nicolaides (Athens, Greece) 285
Electronic structure of coinage metal clusters
K. Balasubramanian (Tempe, AZ, U.S.A.) 291
Taking into account non-dynamical correlation effects in ab initio chemisorption cluster model calculations
F. Illas, J. Rubio, M. Bachs (Barcelona, Spain) and J.M. Ricart (Tarragona, Spain) 315
Structure, energetics and molecule–matrix interactions of molecules substituted into inert clusters and crystals: consistent force field treatment of substitutional defects in imperfect matrices: *trans*-1,2-difluoroethane: Ar_{363}
R. Gunde and Hs.H. Günthard (Zürich, Switzerland) 325
Effective-mass Hamiltonians and wavefunction-matching conditions for abrupt heterojunctions
P. Csavinszky and A.M. Elabsy (Orono, ME, U.S.A.) 337
Magnetism and electronic structure in the (123) and (2212) copper oxides
B. Szpunar, V.H. Smith Jr. and R.W. Smith (Kingston, Ont., Canada) 347
Bonding and structure in the hydrides of groups III–VI deduced from photoionization studies
J. Berkowitz, B. Ruscic, S.T. Gibson, H. Cho and C.A. Mayhew (Argonne, IL, U.S.A.) 363

Author Index 375

Subject Index 376